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P16

Rhombohedral structure observed in the computer simulations of block-copolymer melts

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Diblock copolymer melts show various ordered structures, such as cylinders(C), lamellae(L), and a gyroid structure(G), depending on the temperature and the constitution ratio of two different homopolymers, each consisting of A or B monomers alone. A gyroid structure has a three-dimensional bicontinuous network with I_{a3d} symmetry and negative Gauss curvature.

We carry out computer simulations of diblock copolymer melts, from which we discover a gyroid-like structure between the cylinder phase and the lamellar phase. Our computer simulation of diblock copolymer melts is based on the scheme, *the extended Cahn-Hilliard equations* which enables systems to reach to the most stable state rather easily.

$$\frac{\partial}{\partial t}\phi(\mathbf{r}) = \triangle\left(-A\psi + u\psi^3 - \mathcal{D}\triangle\psi\right) - B\psi, \quad \frac{\partial}{\partial t}\psi(\mathbf{r}) = \phi(\mathbf{r}),$$

in which we have introduced the momentum of the field ϕ as a new term in addition to the ordinary terms in the CH equation.

The results of simulations are shown in Figs. 1-3 in which the illustrations of the surface of a constant ψ value are presented from three different angles.

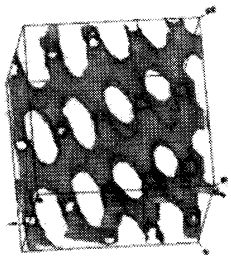

Fig.1

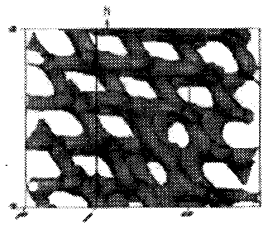

Fig.2

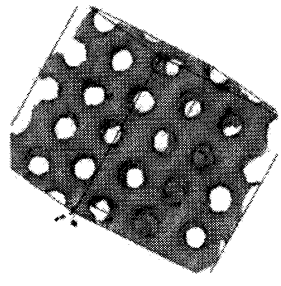

Fig.3

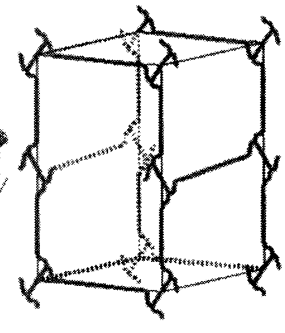

Fig.4

The unit cell of this gyroid-like structure is *rhombohedral* as shown in Fig.4. There are two ways to define the unit cell of rhombohedral-type, i.e., a way in which the a- and b-axis are respectively orthogonal to c-axis, and the other way in which the each length of a- and b- and c-axis is taken to be the same. Here the former way is adopted. In Fig.4, both a- and b-axis are orthogonal to c-axis. The angle between the a-axis and the b-axis is $\pi/3$. The length in the a-direction of a unit cell is the same as that in the b-direction. The ratio of the length in the a-direction (or b-direction) to the length in the c-direction is 1/2.1; in other words, $a : c = 1 : 2.1$, which is found from our computer simulations. From analyzing Fig.4, we can decide the space group symmetry of this gyroid-like structure to belong to $R\bar{3}c$, where the index R represents *rhombohedral*, and $\bar{3}$ represents a three-fold rotoinvertion symmetry, while c means a glide reflection symmetry as to the c-axis.

From the recent studies of scattering experiments by Imai et al., it has been shown that there exists a structure with $R\bar{3}c$ symmetry which appears in the process of L-to-G transition in the nonionic surfactant/water system.

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